

High Production Volume (HPV) Challenge Program

**Data Summary and Test Plan
for**

TMXDI® (META) ALIPHATIC ISOCYANATE

**Isocyanic acid, m-phenylenediiso-propylidene
CAS# 2778-42-9**

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A. INTRODUCTION

On November 22, 1999, Cytec Industries Inc. (Cytec) voluntarily agreed to participate in the Environmental Protection Agency's (EPA) High Production Volume Chemical Challenge Program. By participating in this program, Cytec agreed to assess the adequacy of existing data, design and submit test plans to fill data gaps where necessary and appropriate, provide test results, and prepare summaries of the data characterizing each chemical.

The sponsored chemical addressed in this test plan is Isocyanic acid, m-phenylenediiso-propylidene (CAS# 2778-42-9) (TMXDI).

B. GENERAL SUBSTANCE INFORMATION**Trade Name: TMXDI® (META) ALIPHATIC ISOCYANATE**

Chemical Name: Isocyanic acid, m-phenylenediiso-propylidene

Inventory Names:

Benzene, 1,3-bis(1-isocyanato-1-methylethyl)-
1,3-Bis(1-isocyanato-1-methylethyl)benzene
1,3-bis(1-isocyanato-1-methylethyl)benzene
1,3-Bis(1-isocyanato-1-methylethyl)benzol
1,3-bis(1-isocyanato-1-metiletil)benceno

Other Names:

a,a,a',a'-Tetramethyl-m-phenylenedimethylene diisocyanate
a,a,a',a'-Tetramethyl-m-xylylene diisocyanate
1,3-Bis(a-isocyanatoisopropyl)benzene
Isocyanic acid, a,a,a',a'-tetramethyl-m-xylylene ester
Isocyanic acid, m-phenylenediisopropylidene ester
m-Bis(1-isocyanato-1-methylethyl)benzene
TMXDI
Tetramethyl-m-xylylene diisocyanate

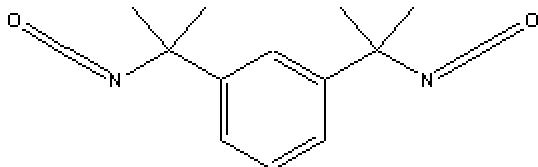
Chemical Abstract Service Registry Number: CAS # 2778-42-9

Common Name: TMXDI

Empirical Formula: C₁₄H₁₆N₂O₂

Molecular Weight: 244.3

Structure:



C. EXPOSURE INFORMATION

1. Use and Exposure Information

Cytec Industries Inc. has produced in excess of 1 million pounds of this material. As such, there are prescribed conditions for its manufacture, processing, distribution, use and disposal. In general, there is low potential for exposure of humans or the environment. In the work place, potential worker exposure is carefully controlled.

2. Manufacture & Processing:

Although diisocyanates are well-known sensitizers, little risk is posed by this chemical. The diisocyanate is manufactured in an essentially closed system with little personnel exposure. Its manufacture is monitored under close technical supervision. Although its vapor pressure is quite low, points of possible exposure are controlled by exhaust systems and, where necessary, carbon filters are used to purify any contaminated air. Protective clothing and respirators are required.

The only worker contact comes from sampling procedures for quality control, and in some instances, during packaging. Exposure would be by skin contact. Inhalation exposure is extremely low due to the use of ventilation and the materials low vapor pressure. Ingestion would not be expected.

In customer applications, this material is used at plants by highly experienced personnel well equipped to handle these materials safely.

TMXDI is not sold directly to the consumer market. This material is reacted into the polymers in which they are added, limiting potential exposure in the finished consumer products.

3. Distribution (Transport):

Since diisocyanates are well known sensitizers, distribution of this material is restricted to customers that are highly experienced and well equipped to handle material of this kind. As is well known, plants handling isocyanates routinely use exhaust systems to minimize hazards due to contaminated air, and where required, protective clothing and respirators are used. Our choice of customers is restricted to companies' well respected in the field and having high standards of industrial hygiene.

This material is transported to our customers in drums, totes, or ISO containers by way of truck or ship with little to no risk to the public or the environment.

4. Uses:

TMXDI aliphatic isocyanate is a versatile aliphatic isocyanate finding broad end-use applicability. Application areas include specialty coatings, aqueous dispersions, automotive coatings, wood coatings, inks, sealants, adhesives, thermoplastic urethanes, and lacquers.

This chemical imparts improved physical properties to polyurethane products, affording higher strength and improved adhesion, appearance, and flexibility, resulting in more durable products.

Common commercial products that may have been made using TMXDI include, fabric and leather finishes, adhesives, automotive paints, printing inks, sealants, and wood coatings. TMXDI poses little to no risk to the end consumer as there is no exposure to TMXDI.

In addition to these uses, TMXDI is FDA approved for use in food-packaging under specific listings in the Code of Federal Regulations (CFR) Title 21-Food and Drugs Chapter I-Food and Drug Administration, Department of Health and Human Services.

Table 1: 21 CFR Sanctions

21 CFR	Section	Definition
PART 175—Indirect Food Additives: Adhesives and Components of Coatings--§175.105 (ADHESIVES)	§175.105	Clears meta-tetramethyl xylene diisocyanate for reaction with one or more of the polyols and polyesters listed in §175.105 and dimethylolpropionic acid and triethylamine, N-methyldiethanolamine, 2-dimethylaminoethanol, 2-dimethyl-amino-2-methyl-1-propanol and/or 2-amino-2-methyl-1-propanol in the production of polyurethane resins intended for use as components of adhesive formulations used in food packaging applications. Cytec Industries Petition Oct. 26, 1993, effective March 12, 1996

5. Disposal:

All waste material is drummed and disposed of by approved waste treatment contractors. This material is not regulated as a RCRA hazardous waste

D. SUMMARY TABLE OF AVAILABLE DATA

CAS# 2778-42-9	Study Date	Results	Data Acceptable
Physical/Chemical Characteristics			
Melting Point	1982	-10°C	Yes
Boiling Point	1982/2002	292 °C (105 °C @ 0.5 mm Hg) 320 °C (est.)	Yes
Vapor Pressure	1986/2002	0.0032 mm Hg @ 25 °C 0.00298 mm Hg @ 25 °C (est.)	Yes
Partition Coefficient	2002	Log K _{ow} = 4.74	Yes
Water Solubility	2002/2002	Insoluble (reacts with water) 5.833 mg/L @ 25 °C (est.); If hydrolysis is rapid, estimated value will be adequate; However, if hydrolysis is slow then definitive study (OECD TG 105) will be conducted	Yes?
Environmental Fate			
Photodegradation	2002	For reaction with hydroxyl radical, predicted rate constant = 10.1332 x 10 ⁻¹² cm ³ /molecule-sec Predicted half-life = 12.666 hours	Yes
Stability in Water	2002	No estimate available, Reacts slowly with water resulting in the formation of insoluble ureas. Definitive study (OECD TG 111) to be conducted to address rate of hydrolysis	No
Transport between Environmental Compartments: Fugacity Level III Model Default assumption: 1000 kg/hr simultaneously released into air, water, and soil.	2002	Air: 0.779% Water: 18.1% Soil: 62.6% Sediment: 18.5%	Yes
Biodegradation	1988	<i>OECD 301D: Closed Bottle Test</i> Not readily biodegradable by this test procedure	Yes
Ecotoxicity			
Acute Toxicity to Fish	1993	<i>OECD 203: Fish Acute Toxicity Test</i> Lepomis macrochirus: NOEC = >52.19 mg/L 96 hr LC50 = >65.88 mg/L (based on exposure to Water Accommodating Fraction, measured by analysis)	Yes

	1986	<i>USEPA 660/3-75-009: Fish Acute Toxicity Test</i> Pimephales promelas NOEC = 0.32 mg/L 96 hr LC50 = 0.67 mg/L (based on material dissolved in acetone)	Yes
Acute Toxicity to Invertebrates	1986	<i>USEPA 660/3-75-009: Daphnia magna Acute Toxicity Test</i> Daphnia magna NOEC = <1.0 mg/L 24-hour LC50 = 6.5 mg/L 48-hr LC50 = 5.2 mg/L (based on material dissolved in acetone)	Yes
Acute Toxicity to Algae	1987	<i>OECD 201: Alga. Growth Inhibition Test</i> Selenastrum capricornutum: NOEC = 0.10 mg/L EbC50 = 0.36 mg/L (based on material dissolved in acetone)	Yes
Mammalian Toxicity			
Acute Toxicity			
Oral	1981	Rat: oral LD50 = 5000 mg/kg	Yes
Dermal	1981	Rabbit: dermal LD50 = >2,000 mg/kg	Yes
Inhalation	1995	Rat: inhalation 4 hr LC50 = 2.7 ppm	Yes
Eye Irritation	1981	Mild Eye Irritant	Yes
Skin Irritation	1981	Moderate Skin Irritant	Yes
Dermal Sensitization	1981	Skin Sensitizer	Yes
Respiratory Sensitization	1984	No Sensitization Response Elicited	Yes
Repeat Dose Toxicity	1987	(28 day inhalation) rat: NOEL = 0.038 ppm	Yes
	1990	NOAEL = 0.15 ppm (90 day inhalation) rat/mice: NOEL = Not Established LOAEL = 0.4 ppm for both species	Yes
Developmental Toxicity		No data	No Data
Reproductive Toxicity	1981	Based on the results of the 90-day repeat dose inhalation study there were no macro or microscopic changes in any of the male or female reproductive organs that could be attributed to exposure to TMXDI. Thus suggestive that at the concentrations tested the material would not be a reproductive toxicant.	Yes
Genetic Toxicity: Gene Mutations	1983	<i>Salmonella typhimurium:</i> Not mutagenic	Yes
Genetic Toxicity: Chromosomal Aberration		No data	No Data

E. TEST PLAN FOR Isocyanic acid, m-Phenylenediiso-Propylidene, CAS# 2778-42-9

CAS# 13893-53-3	Data Available	Data Acceptable	Testing Required
Study	Y/N	Y/N	Y/N
Physical/Chemical Characteristics			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	Y/N
Environmental Fate			
Photodegradation	Y	Y	N
Hydrolysis	-	-	Y
Fugacity	Y	Y	N
Biodegradation	Y	Y	N
Ecotoxicity			
Acute Toxicity to Fish	Y	Y	N
Acute Toxicity to Invertebrates	Y	Y	N
Acute Toxicity to Algae	Y	Y	N
Mammalian Toxicity			
Acute Toxicity	Y	Y	N
Repeat Dose Toxicity	Y	Y	N
Developmental Toxicity	N	No data	Y
Reproductive Toxicity	N	Y	N
Genetic Toxicity: Gene Mutations	Y	Y	N
Genetic Toxicity: Chromosomal Aberration	N	No data	Y